Methylparaben

99-76-3 | DTXSID4022529

Model Performance

Ν	Model	Data

Weighted KNN model

5-fold CV (75%)		Training	Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.84	0.55	0.85	0.53	0.83	0.64	

Model Results

Predicted value: 4.23e-01

Global applicability domain: Inside

Local applicability domain index: 5.35e-01

Confidence level: 7.45e-01

Nearest Neighbors from the Training Set

Image not found

Paraldehyde

Measured: 0.48 Predicted: 4.42e-01

Image not found

2,2-Bis(bromomethyl)-1,3-

propanediol **Measured:** 0.68

Predicted: 5.25e-01

Image not found

2,2,4-Trimethyl-1,3-

pentanediol Measured: 0.0

Predicted: 1.68e-01

Image not found

2-Isopropyl-6-methyl-4-

pyrimidone

Measured: 0.26 Predicted: 3.47e-01

Image not found

2,2-Dimethylpropane-1,3-

diol

Measured: 0.67 Predicted: 6.47e-01